

# Topology of configuration space of mean-field $\phi^4$ model by Morse theory

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In this paper we present the study of the topology of the equipotential hypersurfaces of configuration space of the mean-field  $\phi^4$  model with a  $\mathbb{Z}_2$  symmetry. Our purpose is discovering, if any, the relation between the second-order  $\mathbb{Z}_2$ -symmetry breaking phase transition and the geometrical entities mentioned above. The mean-field interaction allows us to solve analytically either the thermodynamic in the canonical ensemble or the topology by means of Morse theory. We have analyzed the results at the light of two theorems on necessary or sufficient topological-geometrical conditions for phase transitions and symmetry breaking recently proven. This study makes part of a research line based on the general framework of geometric-topological approach to Hamiltonian chaos and critical phenomena.

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## I. INTRODUCTION

Phase transitions are sudden changes of the macroscopic behavior of a physical system composed by many interacting parts occurring while an external parameter is smoothly varied, generally the temperature, but e.g. in a quantum phase transition it is the external magnetic field. From a mathematical viewpoint, a phase transition is a non-analytic point in the partition function emerging as the thermodynamic limit has been performed. The successful description of phase transitions starting from the properties of the microscopic interactions among the components of the system is one of the major achievements of equilibrium statistical mechanics.

From a statistical-mechanical point of view, in the canonical ensemble, a phase transition occurs at special values of the temperature  $T$  called transition points, where thermodynamic quantities such as pressure, magnetization, or heat capacity, are non-analytic functions of  $T$ . These points are the boundaries between different phases of the system. Starting from the exact solution of the 2-dimensional Ising model [25] by Onsager [36], these singularities have been found in many other models, and later developments like the renormalization group theory [20] have considerably deepened our knowledge of the properties of the transition points. Typically, but not necessarily, these singularities are associated with spontaneous symmetry breaking phenomenon, giving rise to symmetry breaking phase transitions (SBPT hereafter). In this paper we consider this case only. But in spite of the success of equilibrium statistical mechanics, the issue of the deep origin of SBPTs remains open, and this motivates further studies of SBPTs.

Consider an  $N$  degrees of freedom system with Hamil-

tonian given by

$$H(\mathbf{p}, \mathbf{q}) = T + V = \sum_{i=1}^N \frac{p_i^2}{2} + V(\mathbf{q}). \quad (1)$$

Let  $M \subseteq \mathbb{R}^N$  be the configuration space. The partition function is by definition

$$\begin{aligned} Z(\beta, N) &= \int_{\mathbb{R}^N \times M} d\mathbf{p} d\mathbf{q} e^{-\beta H(\mathbf{p}, \mathbf{q})} = \\ &= \int_{\mathbb{R}^N} d\mathbf{p} e^{-\beta \sum_{i=1}^N \frac{p_i^2}{2}} \int_M d\mathbf{q} e^{-\beta V(\mathbf{q})} = Z_{\text{kin}} Z_c \end{aligned} \quad (2)$$

where  $\beta = \frac{1}{T}$  (in unit  $k_B = 1$ ),  $Z_{\text{kin}}$  is the kinetic part of  $Z$ , and  $Z_c$  is the configurational part. In order to develop what follows we assume the potential to be lower bounded.  $Z_c$  can be written as follows

$$Z_c = N \int_{v_{\min}}^{+\infty} dv e^{-\beta N v} \int_{\Sigma_{v,N}} \frac{d\Sigma}{\|\nabla V\|} \quad (3)$$

where  $v = \frac{V}{N}$  is the potential per degree of freedom, and the  $\Sigma_{v,N}$ 's are the  $v$ -level sets defined as

$$\Sigma_{v,N} = \{\mathbf{q} \in M : v(\mathbf{q}) = v\}. \quad (4)$$

The  $\Sigma_{v,N}$ 's are the boundaries of the  $M_{v,N}$ 's ( $\Sigma_{v,N} = \partial M_{v,N}$ ) defined as

$$M_{v,N} = \{\mathbf{q} \in M : v(\mathbf{q}) \leq v\}. \quad (5)$$

The set of the  $\Sigma_{v,N}$ 's is a foliation of configuration space  $M$  while varying  $v$  between  $v_{\min}$  and  $+\infty$ . The  $\Sigma_{v,N}$ 's are very important submanifolds of  $M$  because as  $N \rightarrow \infty$  the canonical statistic measure shrinks around  $\Sigma_{\bar{v}(T),N}$ , where  $\bar{v}(T)$  is the average potential per degree of freedom. Thus,  $\Sigma_{\bar{v}(T),N}$  becomes the most probably accessible  $v$ -level set by the representative point of the system.

This fact may have significant consequences on the symmetries of the system and on the analyticity of  $Z_c$

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because of the very complex topology in general of the  $\Sigma_{\bar{v}(T),N}$  which changes while varying  $T$ .

We can make the same considerations for  $Z_{kin}$ , but the related submanifolds  $\Sigma_{t,N}$ , where  $t = \frac{T}{N}$  is the kinetic energy per degree of freedom, are all trivially homeomorphic to an  $N$ -sphere, thus they cannot affect the symmetry properties of the system by topological reasons. Furthermore,  $Z_{kin}$  is analytic at any  $T$  in the thermodynamic limit, so that it cannot entail any loss of analyticity in  $Z$ .

In Sec. II we present a detailed analytical study of the canonical thermodynamic and of the topological changes which occur in the manifolds  $M_{v,N}$  of the mean-field  $\phi^4$  model, which allows a complete and constructive analytical characterization of the topology of the  $M_{v,N}$ 's and also a computation of their Euler characteristic. In Sec. III we present the same study for a case where no SBPT is present, i.e. the  $\phi^4$  model without interaction, in order to compare the two cases and obtain hints towards a general understanding of the general relation between topology changes and SBPTs. In both cases we use Morse theory as a mathematical tool that allows one to study the topology of a manifold  $M$  in terms of the analytical properties of suitable functions (called Morse functions)  $f : M \rightarrow \mathbb{R}$ . The connection between this technique and physics is made by choosing the potential per degree of freedom  $v = \frac{V}{N}$  as our Morse function. In Sec. IV we try to discover any possible relation between the topology and geometry and the  $\mathbb{Z}_2$ -SBPT of the mean-field  $\phi^4$  model at the light of the results obtained in [5, 8–10, 21] where some necessary and sufficient geometric-topological condition for SBPTs are showed.

## II. MEAN-FIELD $\phi^4$ MODEL

The lattice  $\phi^4$  models are a class of models with an  $O(n)$  symmetry for  $n \geq 1$ . We have restricted our study to the  $\phi^4$  model with an  $O(1)$  symmetry (known even as  $\mathbb{Z}_2$  symmetry) and with mean-field (m-f hereafter) interactions, i.e. every degree of freedom interacts with every other. The Hamiltonian is as follows

$$H = T + V = \sum_{i=1}^N \left( \frac{\pi_i^2}{2} - \frac{\phi_i^2}{2} + \frac{\phi_i^4}{4} \right) - \frac{J}{2N} \left( \sum_{i=1}^N \phi_i \right)^2. \quad (6)$$

The  $\pi_i$ 's are the canonically conjugated momenta of the coordinates  $\phi_i$ 's,  $J > 0$  is the coupling constant, and  $N$  is the number of degrees of freedom.

### A. Canonical thermodynamic

In what follows we will disregard the kinetic terms  $\frac{\pi_i^2}{2}$  for the reasons already exposed in the previous section.

The configurational partition function is

$$Z_c = \int d^N \phi e^{-\beta \left( \sum_{i=1}^N V(\phi_i) - \frac{J}{2N} \left( \sum_{i=1}^N \phi_i \right)^2 \right)}, \quad (7)$$

where

$$V(\phi) = -\frac{\phi^2}{2} + \frac{\phi^4}{4} \quad (8)$$

is the local potential. The order parameter, i.e. the magnetization in our case, is

$$m = \frac{1}{N} \sum_{i=1}^N \phi_i, \quad (9)$$

which, introduced in  $Z_c$ , gives

$$Z_c = \int d^N \phi e^{-\beta \left( \sum_{i=1}^N V(\phi_i) - \frac{J}{2} m^2 \right)}, \quad (10)$$

Now, for the sake of completeness, we briefly recall the solution of the thermodynamic by means of m-f theory, but it is available in literature, for example in [15]. M-f interactions imply that the potential is a function of  $m$ , so that we can analytically solve  $Z_c$  by the Hubbard-Stratonovich transformation [20] based on the equality

$$e^{\mu m^2} = \frac{1}{\sqrt{\pi}} \int dy e^{-y^2 + 2\sqrt{\mu} m y}, \quad (11)$$

which, inserted in (10), yields

$$Z_c = \frac{1}{\sqrt{\pi}} \int dy \left( \int d\phi e^{-\beta V(\phi) + \sqrt{\frac{2\beta J}{N}} m \phi} \right)^N e^{-y^2}. \quad (12)$$

After introducing

$$\varphi(m, \beta) = \ln \int d\phi e^{-\beta(V(\phi) + J m \phi)}, \quad (13)$$

and the variable changing  $y = \sqrt{\frac{N\beta J}{2}} m$ , we get

$$Z_c = \sqrt{\frac{N\beta J}{2\pi}} \int dm e^{-N\beta f_c(m, \beta)}, \quad (14)$$

where

$$f_c = -\frac{J}{2} m^2 + \frac{1}{\beta} \varphi(m, \beta) \quad (15)$$

is the configurational free energy per degree of freedom.

Finally, in order to apply the saddle point approximation to calculate  $Z_c$ , we minimize  $f_c$  with respect to  $m$  at fixed  $\beta$  obtaining the spontaneous magnetization  $\bar{m}(\beta)$ . From the latter we get the free energy, the average potential, and the specific heat

$$f_c(\beta) = -\frac{1}{N\beta} \ln Z_c, \quad (16)$$

$$\bar{v}(\beta) = -\frac{\partial}{\partial \beta} f_c(\beta), \quad (17)$$

$$c_v(\beta) = \frac{d\bar{v}}{dT}, \quad (18)$$

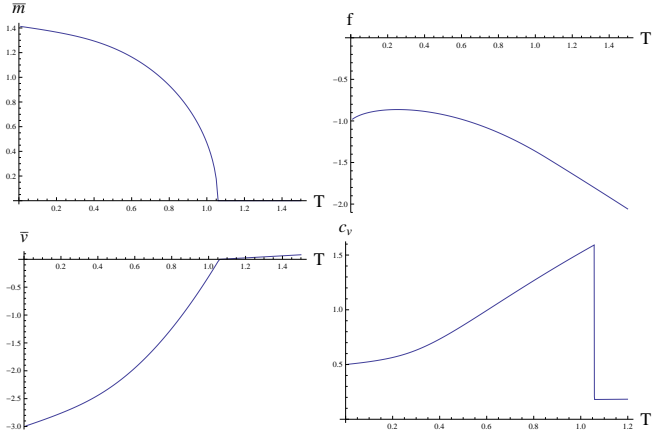


FIG. 1: Mean-field  $\phi^4$  model (6) with coupling constant  $J = 1$ . From left to right, and from top to bottom. Spontaneous magnetization  $\bar{m}$ , free energy  $f$ , specific average potential  $\bar{v}$ , and specific heat  $c_v$  as functions of the temperature  $T$ .

respectively. They are plotted in Fig. 1 as functions of  $T$ . The picture is the well known one of a second-order  $\mathbb{Z}_2$ -SBPT with classical critical exponents.

### B. Topology of the submanifolds $M_{v,N}$ 's by Morse theory

Morse theory allows us to characterize the topology of the submanifolds  $M_{v,N}$  of configuration space  $M = \mathbb{R}^N$  defined in (5) by a Morse function  $f : M \rightarrow \mathbb{R}$ . The last is a function whose critical points are non-degenerate, i.e. such that the Hessian matrix of  $f$  has rank  $N$  at any critical point. For some introductory details of Morse theory we refer to App. A.

The potential  $V : \mathbb{R}^N \rightarrow \mathbb{R}$  is our Morse function. We cannot show in advance that  $V$  is a Morse function, but we have verified that the output of our analysis is a set of isolated critical points. The fact that a critical point is isolated does not imply that it is also non-degenerate, but anyway if the set of critical points are isolated Morse theory can be successfully applied the same, even though the potential  $V$  cannot be properly considered a Morse function. For more information about this delicate question we refer to [34].

The fact that all the critical points are isolated is not surprising, because the set of the Morse functions, or non-properly Morse functions in the sense above-specified, is dense in the set of the smooth functions. Furthermore, the discreteness of the  $\mathbb{Z}_2$  symmetry does not create the problem created by continuous symmetries which entail sets of critical points describing submanifolds of configuration space.

Since in the thermodynamic limit the canonical statistical measure shrinks around the  $\Sigma_{v,N}$  corresponding to the average potential density  $\bar{v}$ , we are interested in the

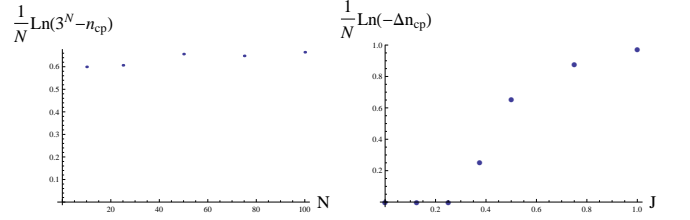


FIG. 2: Mean-field  $\phi^4$  model (6). Left: Estimate of the difference between  $3^N$  and the total amount of critical points  $n_{cp}$  as a function of  $N$  for  $J = 0.5$ . Right:  $\Delta n_{cp} \equiv n_{cp}(J_i) - n_{cp}(J_{i-1})$ , where the  $J_i$ 's are the plotted points, for  $N = 50$ . The total amount of critical points diminishes while increasing  $J$  for  $J > 0.25$ , up to  $J \approx 0.25$  it equals  $3^N$ .

topology of the  $\Sigma_{v,N}$ 's rather than the  $M_{v,N}$ 's. Anyway, the topology of the  $\Sigma_{v,N}$ 's are strictly related to that of the  $M_{v,N}$ 's, in particular if the  $M_{v,N}$ 's are diffeomorphic in an interval  $[a, b]$ , then the same holds also for the  $\Sigma_{v,N}$ 's.

The critical points are the stationary points of  $V$ , i.e. the solutions of  $\nabla V = 0$ , which for the potential of the Hamiltonian (6) takes the form

$$\phi_i^3 - \phi_i - Jm = 0 \quad i = 1, \dots, N, \quad (19)$$

where  $m$  is the magnetization defined in (9). This is a system of  $N$  coupled non linear equations of degree  $3^N$ , thus, if we aspect at most  $3^N$  solutions. Since the equations of the system (19) are all equal, let us omit the index  $i$ , and consider the equation

$$\phi^3 - \phi - Jm = 0. \quad (20)$$

Consider the following cases.

(i);  $|Jm| > \frac{2}{3\sqrt{3}}$ . The equation (20) has one real solution.

(ii);  $|Jm| \leq \frac{2}{3\sqrt{3}}$ . The equation (20) has three real solutions, two of them are coinciding in the limiting case '='.

Case (i) is easier to treat because the system (19) has an unique solution with components  $\phi_i = \phi_0$ ,  $i = 1, \dots, N$ , where  $\phi_0$  is solution of

$$\phi^3 - (1 + J)\phi = 0, \quad (21)$$

therefore, the solutions, with the respective potential values, are

$$\phi_1 = 0, \quad v(\phi_1) = 0, \quad (22)$$

$$\phi_{2,3} = 0, \quad v(\phi_{2,3}) = -\frac{1}{4}(1 + J)^2. \quad (23)$$

Case (ii). The solutions of the system (19) are given by

$$\phi^s = (\underbrace{\phi_1, \dots, \phi_1}_{n_1}, \underbrace{\phi_2, \dots, \phi_2}_{n_2}, \underbrace{\phi_3, \dots, \phi_3}_{N-n_1-n_2}) \quad (24)$$

with all the permutations of  $\phi_1$ ,  $\phi_2$ , and  $\phi_3$ , whose number is the multinomial coefficient

$$(N, n_1, n_2, N - n_1 - n_2)! = \frac{N!}{n_1! n_2! (N - n_1 - n_2)!} \quad (25)$$

for every choice of  $n_1, n_2$  such that

$$0 \leq n_1 \leq N, \quad (26)$$

$$0 \leq n_2 \leq N - n_1. \quad (27)$$

Furthermore,  $\phi_1$ ,  $\phi_2$ , and  $\phi_3$  have to satisfy the constraint

$$Nm = n_1 \phi_1 + n_2 \phi_2 + (N - n_1 - n_2) \phi_3. \quad (28)$$

There are  $\sum_1^{N+1} i = \frac{1}{2}(N+1)(N+2)$  independent equations of the form (28).

To summarize, for a given choice of  $n_1, n_2$  we obtain, if there exist, some solutions of  $m$  which yield solutions of the form (24) with multiplicity  $(N, n_1, n_2, N - n_1 - n_2)!$  and with critical value  $v(\phi^s(m))$ . In the following sections we will see how to calculate the index of every critical point. We have limited to show the results up to  $J = 1$  because some numerical problems makes the results for  $J > 1$  not entirely reliable.

It is easy to prove analytically that all the critical levels of the potential are bounded from above by zero. Start by observing that  $V$  can be written as

$$V = \sum_{i=1}^N \left( \phi_i (\phi_i^3 - \phi_i - Jm) - \frac{\phi_i^4}{4} \right), \quad (29)$$

if  $\phi^s$  is a solution of  $\nabla V = 0$ , the conclusion is immediately reached. In [27] it has been shown the same results for the  $2D$   $\phi^4$  model with nearest-neighbors interaction.

### 1. Index of the critical points

In Morse theory the index of a critical point is the number of negative eigenvalues of the Hessian matrix  $H$ , which for the potential (6) takes the form

$$H_{ij} = \frac{\partial^2 V}{\partial \phi_i \partial \phi_j} = (3\phi_i^2 - 1) \delta_{ij} - \frac{J}{N}. \quad (30)$$

$H$  can be written as  $H = D + B$ , with

$$D_{ij} = (3\phi_i^2 - 1) \delta_{ij}, \quad (31)$$

$$B = -\frac{J}{N} U, \quad (32)$$

where  $U$  is the matrix whose elements equal 1. The eigenvalues of  $D$  read directly on its diagonal, while  $B$  has a unique non-zero eigenvalue of value  $N$  because its rank is 1. Because of the form of  $H$ , we can apply a results based on the Wilkinson theorem which guarantees that, to get the number of negative eigenvalues of  $H$ , if we take the number of the negative eigenvalues of  $D$  we make at most an error of  $\pm 1$ . For more details we refer to [9, 10].

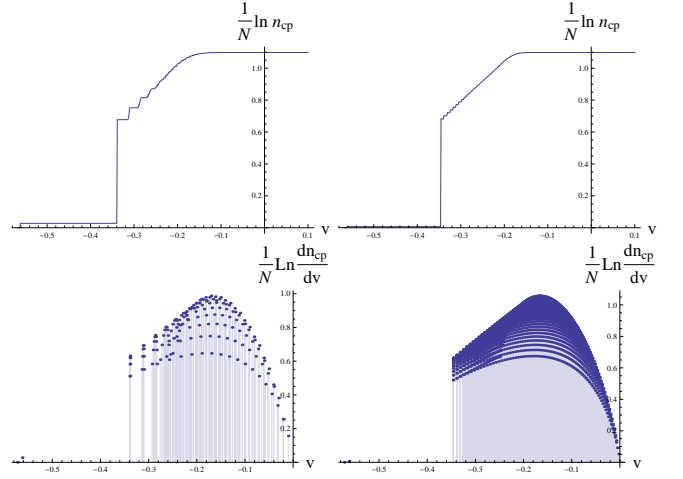


FIG. 3: Mean-field  $\phi^4$  model (6) with  $J = 0.5$ . Top: density of the logarithmic number of critical points as a function of the potential density for  $N = 25$  (left) and  $N = 100$  (right). Bottom: density of the logarithmic density of the number of critical points for  $N = 25$  (left) and  $N = 100$  (right) as a function of the potential density.

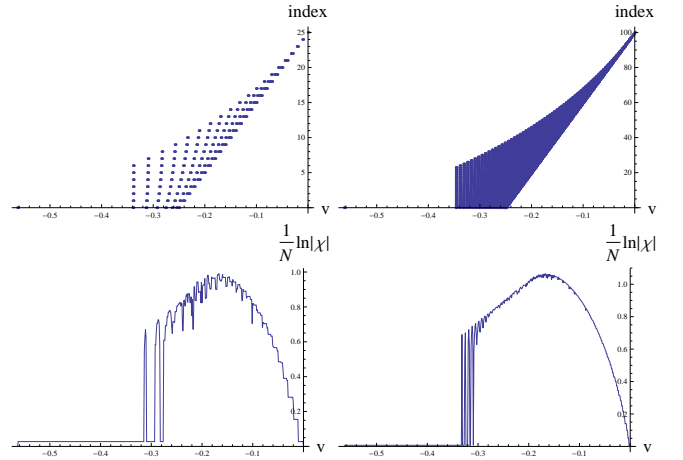


FIG. 4: Mean-field  $\phi^4$  model (6) with  $J = 0.5$ . Left: index of the critical points (top) and the specific logarithmic modulus of the Euler characteristic (bottom) as function of  $v$  for  $N = 25$ . Right: as left for  $N = 100$ .

### 2. Euler Characteristic

The Euler characteristic  $\chi$  is a topological invariant, i.e. a function of a manifold which does not change value if the manifold is deformed without varying its topology.  $\chi$  is defined by the Betti numbers  $b_k$  [37], Morse theory allows us to calculate it for the  $M_{v,N}$ 's by the relation

$$\chi(v, N) \equiv \sum_{k=0}^N (-1)^k b_k(M_{v,N}) = \sum_{k=0}^N (-1)^k \mu_k(M_{v,N}), \quad (33)$$

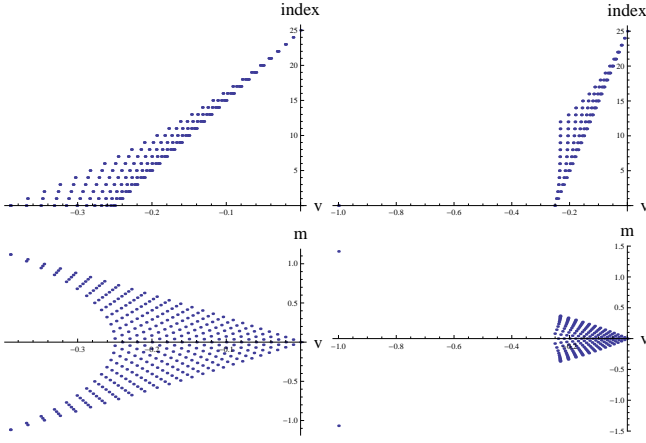


FIG. 5: Mean-field  $\phi^4$  model (6) with  $N = 25$ . Left: index of critical points (top) and magnetization (bottom) as functions of  $v$  for  $J = 0.25$ . Left: as right for  $J = 1$ .

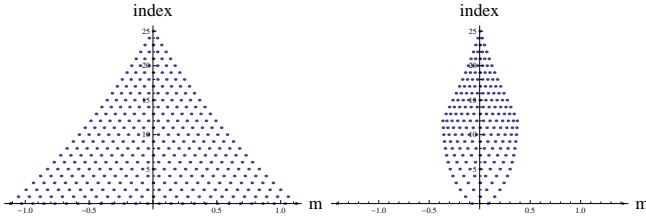


FIG. 6: Mean-field  $\phi^4$  model (6) with  $N = 25$ . Left: index of the critical points as a function of  $m$  at  $J = 0.25$  (left) and  $J = 1$  (right). As  $J$  increases, the magnetization of the critical points shows a tendency to shrink around the  $m$ -axis besides a decrease of the number of critical points.

where the Morse number  $\mu_k$  is the number of critical points of  $M_{v,N}$  that have index  $k$ . In Fig. 4 we have plotted  $\frac{1}{N} \ln |\chi(v)|$  because it approximately does not depend on  $N$ . This is due to the fact that the number of critical points grows exponentially with  $N$ . The modulus appears because  $\chi$  is in general an oscillatory function of  $v$  above and below zero. At  $v > 0$  we have found  $\chi(v) = 1$ . This is coherent with the fact all the critical levels are below zero, because as a consequence  $M_{v,N}$  for  $v > 0$  is homeomorphic to an  $N$ -ball which has  $\chi = 1$ .

### III. $\phi^4$ MODEL WITHOUT INTERACTION

#### A. Canonical thermodynamic

In order to make a confront with a model without SBPT, we have studied the  $\phi^4$  model without interaction. The potential is nothing but that of the Hamiltonian (6) when the interacting terms have been deleted, i.e. as

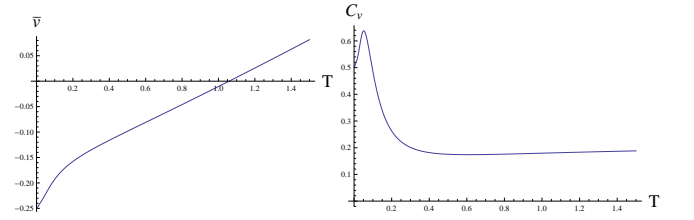


FIG. 7:  $\phi^4$  model without interaction (37). From left to right: average potential density  $\bar{\rho}$  and specific heat  $C_v$  as functions of the temperature  $T$ .

$J = 0$  is set. The configurational partition function is

$$Z_c = \int \prod_{i=1}^N d\phi_i e^{-\beta \sum_{i=1}^N V(\phi_i)} = \left( \int d\phi e^{-\beta V(\phi)} \right)^N, \quad (34)$$

where  $V(\phi)$  is the local potential (8). The analytic solution can be obtained by the following integral

$$\int_0^\infty dz z^{\nu-1} e^{-\gamma z - \alpha z^2} = (2\alpha)^{-\frac{\nu}{2}} \Gamma(\nu) e^{\frac{\gamma^2}{8\alpha}} D_{-\nu} \left( \frac{\gamma}{\sqrt{2\alpha}} \right), \quad (35)$$

where  $D_\nu(z)$  are parabolic cylinder functions. After some algebraic manipulation, we get

$$Z_c = \left( \left( \frac{\beta}{2} \right)^{-\frac{1}{4}} \Gamma \left( \frac{1}{2} \right) e^{\frac{\beta}{8}} D_{-\frac{1}{2}} \left( -\sqrt{\frac{\beta}{2}} \right) \right)^N. \quad (36)$$

No SBPT can occur because the thermodynamic function do not depend on  $N$ , so that the thermodynamic limit cannot generate any emergent behavior.

#### B. Topology of the submanifolds $M_{v,N}$ 's

The potential of the Hamiltonian (6) can be written as  $V = V_{loc} + V_{int}$ , so that the potential of our model is

$$V_{loc} = \sum_{i=1}^N \left( -\frac{\phi_i^2}{2} + \frac{\phi_i^4}{4} \right). \quad (37)$$

As already made for the m-f case, we have to solve  $\nabla V_{loc} = 0$ , which is the following system

$$\phi_i^3 - \phi_i = 0 \quad i = 1, \dots, N. \quad (38)$$

It is immediate to see that the solutions are of the form

$$\phi^s = (\underbrace{\phi_1, \dots, \phi_1}_{n_1}, \underbrace{\phi_2, \dots, \phi_2}_{n_2}, \underbrace{\phi_3, \dots, \phi_3}_{N-n_1-n_2}), \quad (39)$$

where, without loss of generality,  $\phi_1 = 1$ ,  $\phi_2 = -1$  and  $\phi_3 = 0$ .  $n_1$  and  $n_2$  follow the same rule (27). The multiplicity of the solutions for given  $n_1, n_2$  is the same of the m-f  $\phi^4$  model (25).

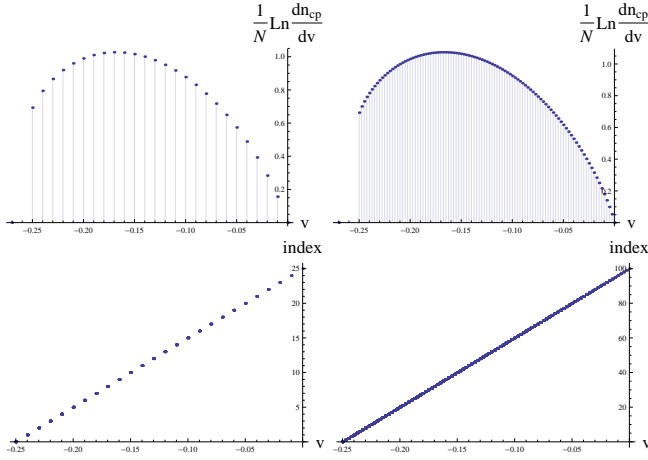


FIG. 8:  $\phi^4$  model without interaction (37). From left to right and from top to bottom. Logarithmic density of critical points per degree of freedom at  $N = 25$ , the same at  $N = 100$ , indexes of the critical points at  $N = 25$ , and the same at  $N = 100$ , as functions of the potential density. Increasing  $N$  does not entail any qualitative difference. The total amount of critical points is fixed at  $3^N$ .

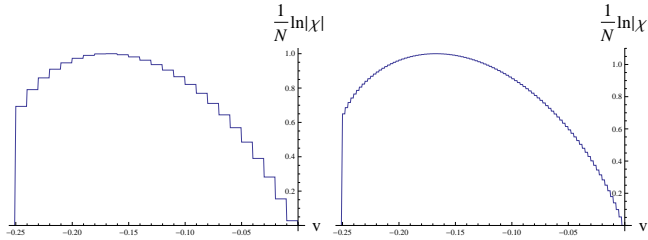


FIG. 9:  $\phi^4$  model without interaction (37). Logarithmic absolute value of the Euler characteristic  $\chi$  per degree of freedom at  $N = 25$  (left), and  $N = 100$  (right) as functions of the potential density.

The Hessian matrix takes the form

$$H_{ij} = \frac{\partial^2 V}{\partial \phi_i \partial \phi_j} = (3\phi_i^2 - 1)\delta_{ij}, \quad (40)$$

so that the index of the critical points is simply  $N - n_1 - n_2$ . For the Euler characteristic, all proceeds as for the m-f  $\phi^4$  model.

#### IV. DISCUSSION OF THE RESULTS

For convenience, in what follows we will consider the  $\Sigma_{v,N}$ 's instead of the  $M_{v,N}$ 's, but they are perfectly equivalent for our purpose. From a topological viewpoint, it is convenient to divide the range of the accessible  $v$ 's of the m-f  $\phi^4$  model in three regions:

(i)  $[v_{min}, v']$ ; the  $\Sigma_{v,N}$ 's are equivalent to the disjoint union of two  $N$ -spheres.  $v_{min} = -\frac{1}{4}(1+J)^2$ , while  $v'$  is

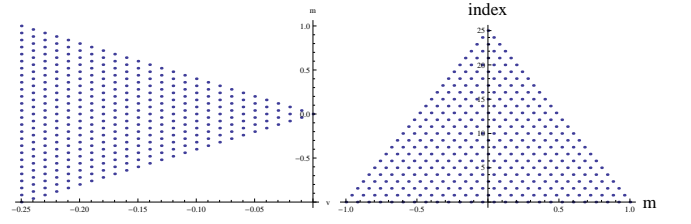


FIG. 10:  $\phi^4$  model without interaction (37) for  $N = 25$ . Left: critical points in the  $(m, v)$ -plane. Right: index of the critical points as a function of  $m$ .

a functions of  $N$  of which some points are plotted in Fig. 11.

(ii)  $[v', 0]$ ; the topology of the  $\Sigma_{v,N}$ 's are dramatically intricate. Simplifying the situation, the interval  $[v', 0]$  plays the role of a critical level which divides region (i) from region (iii).

(iii)  $(0, +\infty]$ ; the  $\Sigma_{v,N}$ 's are equivalent to an  $N$ -sphere.

$v'$  is bounded from above by  $-\frac{1}{4}$ . This is shown in Fig. 11 at least up to  $J = 1.1$ , furthermore it can be analytically proven in the following way. Among the solutions (39) of  $\nabla V_{loc} = 0$ , where  $V_{loc}$  is defined in (37), consider the  $\phi_0^s$ 's for  $n_1 = 0, \dots, N$ , and  $n_2 = n_1$ . The corresponding magnetization is vanishing because it is given by  $m = \frac{n_1 - n_2}{N}$ . Since

$$\nabla V = \nabla V_{loc} - JNm\nabla m, \quad (41)$$

we see that the  $\phi_0^s$ 's are solutions even for  $\nabla V = 0$ . The corresponding value of the potential is  $v = -\frac{1}{4N}(n_1 + n_2)$ . Now distinguish two cases:  $N$  even and  $N$  odd. If  $N$  is even, for  $n_1 = \frac{N}{2}$   $v = -\frac{1}{4}$ , so that the latter is an upper bound of  $v'$ . If  $N$  is odd, for  $n_1 = [\frac{N}{2}]$ , where  $[\cdot]$  is the integer part,  $v = -\frac{1}{4} + \frac{1}{4N}$ , so that  $-\frac{1}{4}$  is an upper bound of  $v'$  even this case.

We conclude that, neither the growing of  $N$ , nor the growing of  $J$  can restrict the critical region (ii). In a further paper we will see how it is possible to reduce it to a unique critical level with an unique critical point of index 1, i.e. a saddle point.

Since as  $J$  increases the total amount of critical points tends to reduce from a maximum of  $3^N$  for  $J < 0.25$  (see Fig. 2, 10), we are led to conjecture that there exists  $J_0$ , eventually dependent on  $N$ , such that for  $J > J_0$  the critical points are the only ones with vanishing magnetization, i.e. with  $n_2 = n_1$ . In other words, the degeneracy on  $n_2$  would be removed by values of  $J$  large enough. Our conjecture is reinforced by a similar result that has been found out in [27, 34] for the 2D  $\phi^4$  model with nearest-neighbors interaction via numerical analysis.

In what follows we will analyze these results at the light of two theorems recently proven.



### A. Theorem on a sufficient topological condition for $\mathbb{Z}_2$ -SBPT

In [5] two straightforward theorems on a sufficient geometric-topological condition for  $\mathbb{Z}_2$ -SBPTs have been shown. For the sake of clarity, in the following considerations we will simplify a little bit the picture.

Consider an  $N$  degrees of freedom Hamiltonian system with a  $\mathbb{Z}_2$ -symmetric, and bonded from below potential. The sufficient condition is as follows: if the  $\Sigma_{v,N}$ 's are made by two disjoint connected components  $A_+$ ,  $A_-$  for  $v \in [v_{\min}, v']$  such that  $A_+$  is the image of  $A_-$  under the  $\mathbb{Z}_2$  symmetry for any  $N$ , then the symmetry is broken for  $\bar{v} \in [v_{\min}, v']$ , where  $\bar{v}(T)$  is the average potential (density) selected by the temperature  $T$ . Furthermore, if there exists a critical potential  $\bar{v}_c$  at which the  $\mathbb{Z}_2$  symmetry breaks, then  $\bar{v}_c \geq v'$  has to hold.

Again, the second theorem states that, if the  $\Sigma_{v,N}$ 's are topologically equivalent to an  $N$ -sphere and ergodic for  $v > v''$  with  $v'' > v'$ , then the  $\mathbb{Z}_2$  symmetry is intact for  $\bar{v} > v''$ , so that a phase transition, meant as a non-analytic point in the magnetization, has to occur as a consequence.

Now will see that the m-f  $\phi^4$  model satisfies the hypotheses of the first theorems, at least for the values of  $N$  considered here, anyway, we have no reasons to doubt that this can hold for every  $N$ . Let us see why. If a double-well potential has the minimum gap between the wells proportional to  $N$ , then it satisfies the hypotheses of the first theorem. Indeed, for the values of the potential comprised between the absolute minimum and the minimum gap between the wells the  $\Sigma_{v,N}$ 's are topological equivalent at least to two disjoint connected components which are non-symmetric under  $\mathbb{Z}_2$  singularly considered. Fig. 11 shows that  $v'$  is proportional to  $N$ , at least for the  $N$ 's considered here. The minimum gap is bounded from below by  $v'$  and from above by 0, so that it is proportional to  $N$ . We can so conclude that the m-f  $\phi^4$  model satisfied the hypotheses of the first theorem.

Now we will show that  $\bar{v}_c \geq v'$  holds for every  $J$ , as requested by first theorem. Fig. 11 shows that the critical average potential  $\bar{v}_c > -\frac{1}{4}$  for  $0 < J < 1$ . To demonstrate that this holds for every  $J$  we resort to the result obtained in [22] which provides that

$$\bar{v}_c = a^2 J^2 - \left(2a^2 - \frac{1}{4}\right) J + \left(\frac{5a^2}{4} - \frac{3}{8} + \frac{1}{64a^2}\right) + O\left(\frac{1}{J}\right), \quad (42)$$

where  $a = \Gamma\left(\frac{3}{4}\right) / \left(\frac{1}{4}\right)$ .

Now we will discuss about the second theorem. If the ergodicity hypothesis were satisfied for all the  $\Sigma_{v,N}$ 's belonging to the region (iii), then the SBPT would be located in the region (ii) for any  $J$ . But since this is not true, the ergodicity cannot be resort to explain the SB for  $v \in (0, \bar{v})$ , despite the fact that the  $\Sigma_{v,N}$ 's are topologically equivalent to an  $N$ -sphere. This means that, besides to the topological one, another SB-mechanism has to be at work. In the next Section we will deep this

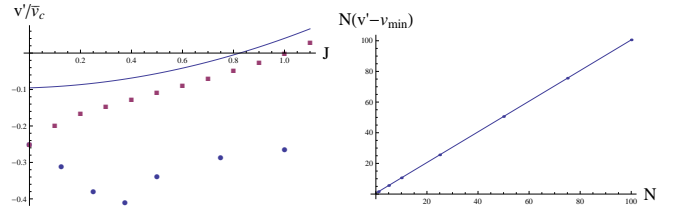


FIG. 11: Left: critical average potential  $\bar{v}$  (squares) and the nearest critical level  $v'$  (disks) above the absolute minimum as functions of the coupling constant  $J$ . The line is the asymptotic expression (42) of  $\bar{v}_c(J)$  at large  $J$ . Right: the interval of  $V$ -values starting from the absolute minimum at which the  $M_{v,N}$  are made by two disjoint  $N$ -spheres as a function of the number of degrees of freedom  $N$ . The line is a linear fit.

question.

### B. Theorem on a necessary topological condition for phase transitions

In [17, 18] a theorem on a necessary topological condition for phase transitions (PT) has been proven. PTs are regarded as a non-analytic point in the thermodynamic functions that arises in the thermodynamic limit. PTs are not necessarily related to symmetry breaking. Simplifying a little bit the picture, the theorem states that if a Hamiltonian system with a potential which is confining, bounded from below, and short-range undergoes a PT, then a topological change has to occur in correspondence of the critical average potential  $\bar{v}_c$  of the PT.

Our results show that  $\bar{v}_c$  may belong either to the region (ii) or to the region (iii). If we are in the second case, then  $\bar{v}_c$  cannot be in correspondence of any critical  $\Sigma_{v,N}$  because they are all topologically equivalent to an  $N$ -sphere. Anyway, this does not affect the theorem because the m-f  $\phi^4$  model is a long-range system which does not satisfy a hypothesis of the theorem.

In [27, 34] the critical points of the 2D  $\phi^4$  model with nearest neighbor interaction have been studied. It has been shown that all the critical points are below zero, like in m-f case. This affects the theorem because the critical potential  $\bar{v}_c$  is unbounded above, so that as it is greater than zero, it cannot be in correspondence to any  $\Sigma_{v,N}$ .

In [21] the authors of the theorem have answered with a generalized version of it where a topological change is only a particular case of a more general necessary condition on the  $\Sigma_{v,N}$ . In particular, the authors extend the concept of diffeomorphicity among manifolds to the concept of *asymptotic diffeomorphicity*, according to which two manifolds can be topologically equivalent at any  $N$  but not asymptotic diffeomorphic as  $N \rightarrow \infty$ . This concept has been successfully applied to the 2D  $\phi^4$  model. We suggest that the same results may be obtained also for the m-f version, and further numerical and analytic

studies in this direction may be a natural extension of this line of research. We suggest that, if this were true, the hypotheses of the theorem may be enlarged to include also long-range potentials.

### C. Euler characteristic

In [8–10] the  $XY$  model in m-f version and without interaction has been studied following the same procedure of this paper. We recall that the m-f  $XY$  model undergoes a second-order  $O(2)$ -SBPT with classical critical exponent, as the m-f interaction requires. The thermodynamic critical average potential is in correspondence of a topological critical level at which a topological change occurs with critical points of all possible indexes, and the graph of the modulus of the Euler characteristic  $\frac{1}{N} \ln |\chi|$  shows a jump. Obviously,  $\frac{1}{N} \ln |\chi|$  has a jump at any critical level, but provided that  $N$  is large enough it can be approximated by a continuous function. In the model without interaction no one of these behaviors shows. At converse,  $\frac{1}{N} \ln |\chi|$  has a continuous shape everywhere.

These results have suggested a strong relation between SBPTs and topological changes, but this scenario does not seem confirmed by the results of the m-f  $\phi^4$  model founded out here.  $\frac{1}{N} \ln |\chi|$  shows a jump at  $v'$  followed by a very intricate shape and by an angular point at  $v = 0$ .  $v'$  never corresponds to the thermodynamic critical average potential, while  $v = 0$  corresponds only for a particular choice of  $J$ . Worst, this shape is showed even by the model without interaction where no SBPT occurs, even though the graph is more regular. We conclude that the scenario depicted by the m-f  $XY$  model is a particular case without any particular significance from a viewpoint of the relation between SBPT and topology of configuration space.

## V. CONCLUDING REMARKS

In this paper we have analytically characterized the topology of the  $M_{v,N}$ 's of the m-f  $\phi^4$  model and the same model without interaction by means of Morse theory. Then, we have tried to discover any possible link with the  $\mathbb{Z}_2$ -SBPT occurring in the m-f  $\phi^4$  model. From a topological viewpoint we have not spotted any qualitative difference between the two models. The critical levels remain confined in an interval of the potential which is  $[-\frac{1}{4}, 0]$  for the model without interaction and  $[v', 0]$  for the m-f model, where  $v' \rightarrow -\frac{1}{4}^-$  as  $J$  increases.

Despite the huge number of critical points growing as  $3^N$ , but decreasing at the increasing of  $J$ , in our opinion all that critical points do not have any particular significance except that to separate the region (i), where the  $M_{v,N}$ 's are homeomorphic to two disjoint  $N$ -balls, from the region (iii), where  $M_{v,N}$ 's are homeomorphic to an  $N$ -ball alone. This is true only in the m-f  $\phi^4$  model, where the potential is double-well with the two absolute

minima separated by a minimum gap proportional to  $N$ . This is the effect of the m-f interaction and it is the very peculiar difference between the two models. Indeed, the absolute minima of the model without interaction are  $2^N$  and remain located at  $v = -\frac{1}{4}$ .

We wonder weather the scenario of the m-f  $\phi^4$  model may be transferred to any short-range version. In our opinion the answer is negative, because a double-well potential with minimum gap proportional to  $N$  implies a non-concave graph of the microcanonical entropy  $s(v, m)$ , while in a short-range system it must be concave or non-strictly concave in the presence of a phase transition. Furthermore, it can be shown that for a short-range  $d$ -dimensional Ising model the minimum gap is proportional to  $N^{\frac{d-1}{d}}$  in the limit of large  $N$ .

Nevertheless, in [34] the authors have found the potential of the nearest-neighbor  $2D$  version to have only three critical points, i.e. a saddle at the 0-level set and two absolute minima at a level set proportional to  $-N$ , for values of the coupling constant  $J$  large enough. Let  $J_0(N)$  be the minimum value of  $J$  for which the critical points are only three at fixed  $N$ . It turns out that  $J_0(N)$  allegedly goes as  $N^2$ , so that, starting from  $J_0(N)$  and  $N$ , new critical points, whose critical levels belong to  $(v_{min}, 0)$ , necessarily arise while increasing  $N$ . This is not a proof that the minimum gap cannot be proportional to  $N$ , but if this were not true, then the minimum gap should be necessarily proportional to  $N$  even in the nearest-neighbor  $2D$  version.

Another remarkable fact is that the SBPT occurs even in correspondence of  $\Sigma_{v,N}$ 's which are topological equivalent to an  $N$ -sphere. This means that a further SB mechanism must exist besides the topological one working for  $v \in [v', 0]$ . In other words, the ergodicity of a  $\Sigma_{v,N}$  cannot be guaranteed by the only assumption that it is homeomorphic to an  $N$ -sphere, as is already arisen from the  $2D$   $\phi^4$  model. Further studies about the asymptotic diffeomorphicity [21] of the  $\Sigma_{v,N}$  in correspondence to the critical point may be a natural line of future research. To conclude, we hope that this work may give useful hints to deepen our understanding of the role of geometry and topology of configuration space in phase transitions phenomenon.

## Appendix A: A glance at Morse theory

Morse theory links the topology of a given manifold  $M$  with the properties of the critical points of smooth functions defined on it. Two manifold  $M$  and  $M'$  are topologically equivalent if they can be smoothly deformed one into the other, i.e. if there exists a *diffeomorphism*  $\psi$  that maps  $M$  into  $M' = \psi(M)$ . Here we consider only compact, finite-dimensional manifolds, but most of the results can be extended to non-compact manifolds. The key ingredient of Morse theory is to consider the manifold  $M$  as decomposed into the *level sets* of a function  $f$ . We



recall that the  $v$ -level set of  $f : M \rightarrow \mathbb{R}$  is the set

$$f^{-1}(a) = \{x \in M : f(x) = a\}. \quad (\text{A1})$$

$M$  being compact, any function  $f$  has a minimum  $f_m$  and a maximum  $f_M$ , so that one can build  $M$  starting from  $f^{-1}(f_m)$  and then adding continuously to it all other level surfaces up to  $f^{-1}(f_M)$ . Further, we define the 'part of  $M$  below  $a$ ' as

$$M_a = \{x \in M : f(x) \leq a\}. \quad (\text{A2})$$

As  $a$  is varied between  $f_m$  and  $f_M$ ,  $M_a$  describes the whole manifold  $M$ .

For our purposes, we need to restrict the class of functions into the class of *Morse functions*, which are defined as follows. A point  $x_c$  is called a *critical point* of  $f$  if  $\nabla f(x_0) = 0$ , while the value  $f(x_0)$  is called a *critical value*.  $f$  is called a Morse function on  $M$  if its critical points are non-degenerate, i.e., if the Hessian matrix of  $f$  at  $x_c$ , whose elements in local coordinates are

$$H_{ij} = \frac{\partial^2 f}{\partial x_i \partial x_j}, \quad (\text{A3})$$

has rank  $n$ , where  $n$  is the dimension of  $M$ . As a consequence, one can prove that the critical points  $x_c$  of a Morse function, and also its critical values, are isolated. It can be proved also that the set of the Morse functions are dense in the space of the smooth functions from  $M$  to  $\mathbb{R}$ . A level set is called *critical level* if there is at least a critical point belonging to it.

If the interval  $[a, b]$  contains no critical values of  $f$ , then the topology of  $f^{-1}([a, b])$  does not change for any  $v \in (a, b]$ . This result is sometimes called the *noncritical neck theorem*.

If the interval  $[a, b]$  contains critical values, the topology of  $f^{-1}[a, b]$  changes in correspondence with the critical values themselves, in a way that is completely determined by the properties of  $H$  at the critical points. The number of negative eigenvalues of  $H$ ,  $k$ , is the *index* of the critical point. The change undergone by the submanifolds  $M_a$  as a critical level is passed is described using the concept of 'attaching handles'. Suppose that the critical level contains a critical point of index  $k$ . We define a  $k$ -handle  $H^{n,k}$  in  $n$  dimensions ( $0 \leq k \leq n$ ) as a product of two disks, one  $k$ -dimensional and the other  $(n - k)$ -dimensional:

$$H^{n,k} = D^k \times D^{n-k}. \quad (\text{A4})$$

Having defined handles, we can state the main result of Morse theory. Let  $\phi$  a smooth embedding  $\phi : \mathbb{S}^k \times D^{n-k} \rightarrow \partial M$  ( $\mathbb{S}^k$  is a  $k$ -sphere). Then one can build the topological space  $M \cup_\phi H^{n,k}$ , i.e.  $M$  with a  $k$ -handle attached by  $\phi$ . This procedure admits a generalization to the simultaneous attachment of  $m$   $n$ -dimensional handles  $H_1^{n,k_1}, \dots, H_m^{n,k_m}$  of indexes  $k_1, \dots, k_m$ .

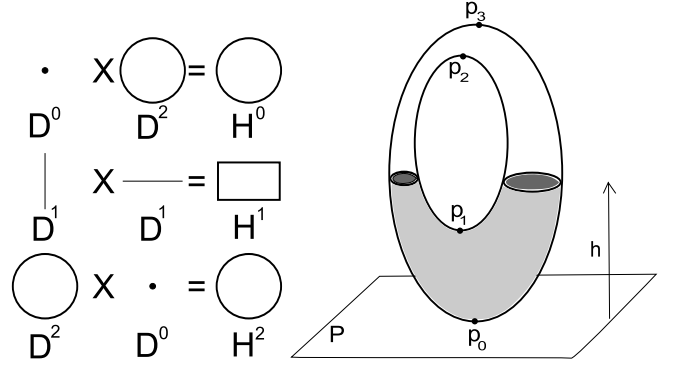


FIG. 12: Left: 2D handles;  $H^0$  is the product of a 0-disk and a 2-disk, so that it is a 2-disk. The same for the other two cases. Right: an example of a 2D-torus. The height  $h$  with respect to the plane  $P$  is the Morse function,  $M_h$  is the gray-colored part of the torus,  $p_i$  for  $i = 0, 1, 2, 3$  are the critical points of indexes  $k = 0, 1, 1, 2$ , respectively. The topology of the whole torus is reconstructed by attaching handles  $H^0, H^1, H^1, H^2$ , respectively at the critical levels corresponding with  $p_i$  for  $i = 0, 1, 2, 3$ .

## Appendix B: Mean-field $|\phi|^3$ model

Equation (28) is equivalent to a 5th degree equation in the magnetization  $m$ . Only numerical solutions are available for this equation. In order to check the results obtained here, we have introduced a slight modification in the m-f  $\phi^4$  model to obtain an equation (28) solvable analytically, i.e. of a degree less or equal to the 4th. The goal has been get by lowering the degree of the local potential by one unit, i.e. by substituting the quartic term by a cubic term where the modulus has been added to conserve the  $\mathbb{Z}_2$  symmetry, so that the local potential takes the form

$$V(\phi) = -\frac{\phi^2}{2} + \frac{|\phi|^3}{3}. \quad (\text{B1})$$

$\nabla V = 0$  becomes

$$\pm \phi_i^2 - \phi_i - Jm = 0, \quad i = 1, \dots, N, \quad (\text{B2})$$

where the sign  $+$  has to be taken if  $\phi \geq 0$ , while the  $-$  if  $\phi \leq 0$ . The solutions are

$$\phi_1 = \frac{1 + \sqrt{A_+}}{2}, \quad (\text{B3})$$

$$\phi_2 = \frac{-1 + \sqrt{A_-}}{2}, \quad (\text{B4})$$

$$\phi_3 = \frac{-1 - \sqrt{A_-}}{2}, \quad (\text{B5})$$

where  $A_{\pm} = 1 \pm Jm$ . By inserting in (28) we get

$$am + b = c\sqrt{A_+} + d\sqrt{A_-}, \quad (\text{B6})$$

where the coefficients  $a = 2N$ ,  $b = N - 2n_1$ ,  $c = n_1$ , and  $d = -N + n_1 + 2n_2$  have been introduced. The last

equation is equivalent to

$$((am + b)^2 - c^2 A_+ - b^2 A_-)^2 = 4c^2 d^2 A_+ A_-, \quad (\text{B7})$$

which is a 4th degree equation in  $m$ , q.e.d..

The results do not show any qualitative difference with respect to the m-f  $\phi^4$  model, neither in the canonical thermodynamic, nor in the topology of the  $v$ -level sets. All the considerations made in Sec. II for the m-f  $\phi^4$  model can be perfectly transferred to the m-f  $|\phi|^3$  model.

## Acknowledgments

The most part of the work in this paper is contained in my Master's thesis [4], hence I would like to warmly thank the supervisor L. Casetti. Furthermore, I would like to thank also M. Pettini for priceless discussion, suggestions, and for having created and continuously supported this line of research.

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